

Analytical universal antiproton-atom interaction potential

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Low-energy (keV or less) antiprotons moving or scattering in ordinary matter is strongly affected by the interaction potential between the antiproton and the atoms. This interaction can be modeled by using potentials that have been obtained in quantum chemical calculations of the interaction between an antiproton and an atom with electron screening. To determine the interactions of antiprotons with any element, we here develop a universal antiproton-atom interaction potential. The potential is constructed by fitting a universal functional form to 14 pair-specific antiproton-atom potentials calculated with quantum chemical approaches and tested against three pair-specific potentials that were not part of the fit. We also report pair-specific screened antiproton-atom potentials for 17 elements, five of which are constructed in this work. By performing molecular dynamics simulations of the antiproton transmission through thin films, we show that the universal potential yields almost as good agreement with experiments as simulations carried out with the pair-specific potentials.

I. INTRODUCTION

The scattering and nuclear stopping power of ions of ordinary matter with kinetic energy in the keV to MeV range is determined by the repulsive interatomic potential [1–6]. The repulsive potential leads to a high-energy interaction between an energetic ion with atomic number of Z_1 and with gas or material atoms with atomic number of Z_2 . For antiprotons, the scattering and nuclear stopping power is analogously determined by the fully attractive antiproton-atom potential [7]. Recently, quantum chemical methods were used to calculate pair-specific interaction energies between antiprotons and atoms [7, 8]. However, such potentials are not available for all antiproton-atom pairs, which limits the number of materials for which antiproton scattering and stopping simulations can be performed. Having potentials for all atoms would be valuable since antiproton experiments are carried out with a wide range of different materials in the stopping foils and chambers (eg. Refs. [9–14]).

For ordinary matter, nuclear stopping calculations are possible for any ion in any material due to universal repulsive potentials, many of which have been developed over the last century [1, 15]. The most recent ones have been developed by Ziegler, Biersack and Littmark (ZBL) [4], and by Zinoviev [16]. These potentials were developed by fitting a universal screening length and exponential screening function to quantum-mechanically calculated interaction energies for pairs of atoms (Z_1, Z_2).

We are not aware of a similar effort having been carried out for antiprotons.

In this work, we develop a universal antiproton-atom interaction potential as a function of the atomic number Z_2 of the ordinary matter and with $Z_1 = -1$ for antiprotons. We used quantum mechanical calculations at the Hartree-Fock level to determine pair-specific interaction energies for 5 elements (He, Li, Fe, W, and Pb) to complement the 12 antiproton-atom interaction potentials previously calculated by us [7, 8]. We use pair-specific and universal potentials in molecular dynamics simulations of antiproton transmission through foils, which can be compared to available experimental data.

This paper is organized as follows. In Sec. II, we present the quantum chemical method, the functional form of the universal potential, and describe the fitting approach. In Sec. III, we present the results obtained using the pair-specific and universal fits. In Sec. IV, we compare the binary collision scattering behavior of the pair-specific and universal potential, and in Sec. V, we compare the results of the simulations to experimental data. The results are discussed and summarized in Sec. VI.

II. METHODS

A. Quantum chemical methods

The interaction potentials were calculated as a function of the distance between a negative point charge of $-1e$ and Fe, W and Pb atoms at the scalar relativistic Dirac-Fock level using Turbomole [17–21]. We used the uncontracted ANO-RCC (21s15p10d6f) basis set for Fe,

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(24s21p15d11f) for W and (25s22p16d12f) for Pb.[22] The g and h basis functions were removed from the standard basis sets. For H, He and Li, we used the uncontracted def2-TZVP basis sets [23]. The hydrogen def2-TZVP basis set was used for the antiproton [23]. A finite nucleus with Gaussian distribution was used in the scalar relativistic calculations [24].

B. Functional form for pair potential

As in previous works [4, 7, 8], we describe the interaction potential between particles as a screened Coulomb potential of the form

$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r} \phi(r). \quad (1)$$

Here $Z_1 = -1$ is the elementary charge of the antiproton and Z_2 the elementary charge of the nucleus, whose potential energy is determined, and r is the separation between the antiproton and the center of the nucleus of the ordinary matter atom. Like in Refs. 7 and 8, we define the screening function $\phi(r)$ as a sum of four exponential functions

$$\phi_{\text{fit}}(r) = b_1 e^{a_1 r} + b_2 e^{a_2 r} + b_3 e^{a_3 r} + b_4 e^{a_4 r}. \quad (2)$$

The coefficient of the last term is set to $b_4 = 1 - b_1 - b_2 - b_3$ to ensure a pure Coulomb potential in the limit where $r \rightarrow 0$, *i.e.*, $\phi_{\text{fit}}^{\text{exp}}(r) = 1$ for $r = 0$. The parameters were obtained by fitting the function to the data obtained in the quantum chemical calculations.

C. Functional form for universal potential

Since the radius of the electron density of atoms increases with increasing atomic number Z , the construction of universal repulsive potentials conventionally uses a screening length a_u that is smaller for heavy atoms [1, 4, 15, 16]. The universal antiproton potential of any element Z_2 is based on the Coulomb potential (eq. 1). The generalized screening function depends on the reduced radius $r_{\text{red}} = r/a_u$, where the universal screening length a_u is a function of Z_2 :

$$V(Z_2, r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r} \phi_{\text{uni}}(r/a_u(Z_2)). \quad (3)$$

To construct the screening-length of the universal potential, we used the ZBL expression [4] $a_u = 0.8845 \cdot 0.529/(Z_1^{0.23} + Z_2^{0.23})$ as the starting point. Since there is no *a priori* reason why it would depend on Z_2 in the same way as for ordinary matter, we decided to fit the exponent. As the term $Z_1^{0.23}$ is not meaningful for antiprotons, we replaced this with a fitted constant u_2 . We also replaced the constant $0.8845 \cdot 0.529$, which has no

clear physical meaning, with a fitted constant u_1 . The expression for the screening length is

$$a_u(Z_2) = \frac{u_1}{u_2 + Z_2^{u_3}}. \quad (4)$$

For the universal screening function $\phi_{\text{uni}}(r_{\text{red}})$, we used the expression given in eq. 2, with the fitted constants a_i and b_i .

D. Pair-specific fits

The pair-specific expressions were fitted to the quantum chemically calculated data using the Levenberg-Marquardt method of least squares and the gradient search method approximation for nonlinear fitting [25, 26]. In practice, this was implemented in a fitting program `fitf` based on the `curfit` subroutine in Ref. [26]. The `fitf` code is provided in the online supplementary materials.

The individual Φ_i values of the screening function at a distance of r_i from the atomic nucleus are taken from a Gaussian distribution with a mean value of $\phi(r_i)$ and a standard deviation of σ_i . For a Gaussian distribution, the probability of obtaining the calculated values is

$$P_i = \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{\Phi_i - \phi(r_i)}{\sigma_i} \right)^2 \right]. \quad (5)$$

Hence, the probability of obtaining a set of “measured data points” (in our case quantum chemical simulation data) is

$$P = \prod_{i=1}^N P_i. \quad (6)$$

The purpose of this approach is to choose the parameters of $\phi(r)$ such that the probability is maximized, implying that the sum in the exponent, often referred to as the goodness-of-fit parameter χ^2 , is minimized. Since the fit function is not linearly dependent on the fitted parameters, analytical methods cannot be used. The gradient-search method used is based on a numerical estimation of the gradient of χ^2 . When searching for the minimum of χ^2 , we use the direction of the steepest descent method.

Due to the deterministic nature of the calculated data points, they do not have any statistical errors. As the aim is to obtain an as good as possible fit to all data points, we used the approach of selecting arbitrary error values for the fit. Then we used the root-mean-square deviation (E_{rms}) and the mean error Δ , calculated as

$$E_{\text{rms}} = \sqrt{\frac{\sum (\varphi_{\text{fit},i} - \varphi_{\text{cal},i})^2}{N}}, \quad (7)$$

and

$$\Delta = \frac{1}{N} \sum \left(\frac{\varphi_{\text{fit},i}}{\varphi_{\text{cal},i}} - 1 \right). \quad (8)$$

to assess the accuracy of the fits. Here, N is the total number of data points, φ_{cal} the quantum chemically calculated values for the screening function and φ_{fit} the fitted value corresponding to the same distance from the nucleus as the calculated value. This error analysis was independent of the fitting process.

After testing several types of error values, we found that running the fitting algorithm with a 1% error in the values of the screening function corresponding to an interatomic distance $r < 0.2 \text{ \AA}$ and a 10% error for values of the screening function corresponding to an interatomic distance $r > 0.2 \text{ \AA}$ were suitable to obtain good fits with low E_{rms} and Δ values defined in eqs. 7 and 8. This error was used for the new pair-specific screening functions and to re-optimize the screening functions in Ref. [7], with the exception for the pair-specific fit for hydrogen. The pair-specific screening functions in Ref. [8] (fits for Cu, Ag, Au) were not re-optimized. They are reported here for comparison with the universal fit.

E. Universal fit

The fitting code `fitf` was extended for the universal fit. Instead of using a 1-dimensional vector r_i as the dependent variable, the dependent variables were gathered in a 2-dimensional matrix $(r_i, Z_{2,i})$, where each data point i obtained at a distance r_i in the quantum chemical calculations was paired with the atomic number $Z_{2,i}$. Thus, one single optimization could be used to fit the $\phi_{\text{uni}}(r, Z_2)$ values of all elements belonging to the dataset. The rest of the fitting procedure was the same as described in subsection IID. The generalized fitting code `fitf2D` is provided in the online supplementary materials.

First, the same errors as in the pair-specific fit were used. However, since this approach did not yield reasonable accuracy, we decided to use the same weight for all data points. We estimated the standard error of the parameters in the universal fit with jackknife resampling [27]. The resampling was done by excluding the data from one atom and repeating the least-square fitting method for the rest of the dataset. This procedure was repeated for the entire dataset. The jackknife estimate of the standard error is

$$SE = \sqrt{\frac{1}{n(n-1)} \sum_i (x_i - \bar{x})^2}, \quad (9)$$

where $\bar{x}$ is the mean of the parameters fitted to the resampled data,

$$\bar{x} = \frac{1}{n} \sum_i x_i, \quad (10)$$

and x_i is the value of the parameter fitted to the data excluding the data for atom i . In our case, n is the number of different pair-specific antiproton-atom potentials used

in the fitting of the universal potential. This approach was repeated for all parameters.

III. RESULTS

A. Pair-specific fits

The parameters of the pair-specific screening functions are shown in table I together with the calculated errors. For completeness, the results of the fit are provided for the previously fitted potentials [7, 8] and the ones determined in this work (He, Li, Fe, W, Pb). The table also includes results of the error analysis (Δ and E_{rms}). The parameters for Al are also new, since we obtained a considerably better fit than the previously reported one [28]. For the other parameters reported in Ref. 7, we reproduced the parameters to at least 4 significant figures and could not find significantly improved fits. The new screening functions for Fe and Pb reported in table I were obtained by fitting with the same errors as for the rest of the pairs.

The fitted pair-specific screening functions, the screening functions reported in Ref. 8, and the quantum chemically calculated data are plotted in Fig. 1 as a function of the distance r between the nucleus and the antiproton.

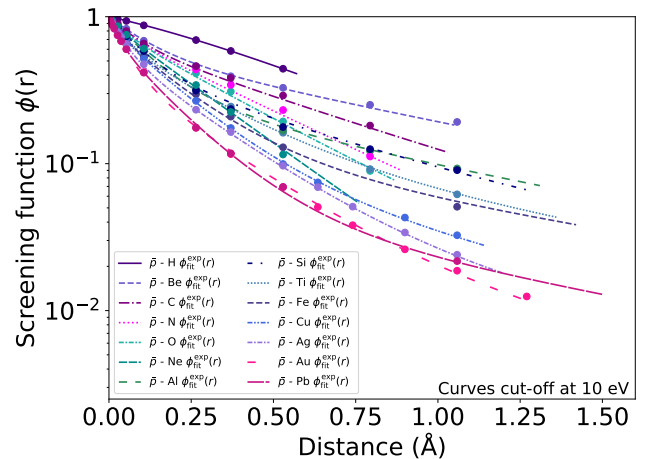


FIG. 1. The pair-specific screening functions (lines) and data (points) plotted as a function of the internuclear distance. The dots indicate calculated data, to which we fitted the exponential screening function. Only screening functions corresponding to a potential energy above 10 eV are included in the figure. We use this cut-off to make the figure comparable to the other figures.

In Fig. 2, the screening function for the Al, Si, Pb, Fe and Cu atoms are shown for a larger internuclear range. We note that the pair-specific screening functions are accurate also at potential energies below 10 eV.

The insert of Fig. 2 shows the screening function for Cu up to a distance of 26.5 Å. For copper, we had more data points in the low energy region, which might explain the

TABLE I. Pair-specific potential parameters for all element pairs, obtained by fitting the screening functions to the data, where "univ" stands for the error of the universal KNGS potential. The a_i coefficients have units of $1/\text{\AA}$ and the b_i coefficients are unitless. The asterisk (*) denotes that the fit differs from the previously reported one, and ** denotes a new pair-specific fit. $\dagger$ denotes elements that were not part of the universal potential fit. Headings X_n refers to the n -th term in the screening function. When estimating the error of the universal KNGS potential, only data corresponding to a potential energy of 10 eV or higher have been taken into account. Eqs. 8 and 7 were used to calculate the errors for the pair-specific fit and the universal potential. In the calculations of the errors of pair-specific fits for He, Li and W, data for interatomic distances larger than 30 $\text{\AA}$ was disregarded to make the errors comparable to the ones of the other atom-antiproton pairs.

El.	Z_2	X	X_1	X_2	X_3	X_4	$\Delta(\%)$	$E_{\text{rms}}(\%)$	$\Delta_{\text{univ}}(\%)$	$E_{\text{rms,univ}}(\%)$
H	1	b	10.688	0.000319357	0.0059701	$1 - b_1 - b_2 - b_3$	0.02032	0.09005	-3.896	4.122
		a	-2.60175	-0.231507	-0.689763	-2.75173				
He**,†	2	b	0.0000123442	1.07018	0.00191974	$1 - b_1 - b_2 - b_3$	0.4739	0.4871	4.929	4.462
		a	-0.0918336	-3.09928	-0.533485	-17.7977				
Li**,†	3	b	0.000506573	0.325888	0.0146870	$1 - b_1 - b_2 - b_3$	-0.05636	0.6289	0.3136	2.134
		a	-0.0588608	-0.582430	-0.199702	-4.92311				
Be	4	b	0.00466484	0.525641	0.027757	$1 - b_1 - b_2 - b_3$	-0.274	0.5094	-6.297	3.309
		a	-0.217729	-1.11801	-0.48179	-7.7278				
C	6	b	0.0380302	0.318996	0.638666	$1 - b_1 - b_2 - b_3$	-0.5524	0.6114	-4.563	2.4
		a	-0.612817	-11.2902	-1.84257	-0.193946				
N	7	b	0.0181678	0.765059	0.216198	$1 - b_1 - b_2 - b_3$	-0.5693	0.7956	0.5088	1.106
		a	-0.824271	-2.52968	-14.7289	-0.242982				
O	8	b	0.0264826	0.790077	0.182093	$1 - b_1 - b_2 - b_3$	-0.335	0.5526	3.907	1.193
		a	-0.847469	-2.906	-17.2312	-0.200413				
Ne	10	b	0.000113387	0.00617107	0.116765	$1 - b_1 - b_2 - b_3$	0.09758	0.3176	9.849	3.199
		a	-0.253027	-0.994693	-24.0586	-3.74468				
Al*	13	b	0.00126049	0.0244898	0.272433	$1 - b_1 - b_2 - b_3$	0.4108	0.4728	-2.474	1.775
		a	-0.0965099	-0.413398	-1.21478	-7.50997				
Si	14	b	0.00547494	0.360324	0.091372	$1 - b_1 - b_2 - b_3$	0.7264	0.7091	-3.841	1.697
		a	-0.19811	-1.99426	-0.79267	-9.71705				
Ti	22	b	0.00226208	0.574763	0.135421	$1 - b_1 - b_2 - b_3$	-0.1408	0.1934	-7.614	1.841
		a	-0.247931	-3.83816	-0.924926	-18.5785				
Fe**	26	b	0.00440192	0.687446	0.13132	$1 - b_1 - b_2 - b_3$	-0.7617	0.363	-2.481	0.7576
		a	-0.257709	-5.12267	-0.933633	-26.4429				
Cu	29	b	0.00176877	0.715859	0.106417	$1 - b_1 - b_2 - b_3$	-2.553	0.1305	2.41	0.4135
		a	-0.333232	-5.1509	-1.28497	-27.2726				
Ag	47	b	0.000985221	0.563975	0.0374024	$1 - b_1 - b_2 - b_3$	-0.4052	0.3102	-1.835	0.6777
		a	-0.260267	-3.91193	-0.944955	-19.0258				
W**,†	74	b	0.000917804	0.547161	0.0418203	$1 - b_1 - b_2 - b_3$	-0.03430	0.5083	-6.935	0.4664
		a	-0.190540	-4.50375	-0.833354	-21.2782				
Au	79	b	0.000854978	0.400538	0.0380799	$1 - b_1 - b_2 - b_3$	-0.05135	0.5915	-2.709	0.415
		a	-0.322095	-3.86192	-1.21461	-17.2175				
Pb**	82	b	0.00209028	0.649905	0.0585822	$1 - b_1 - b_2 - b_3$	-0.01544	0.3569	-2.447	0.5141
		a	-0.221506	-5.81395	-1.09795	-29.5424				

large Δ error presented in table I. This should not affect the usefulness of the pair-specific potential for Cu, since the screening functions at internuclear distances much longer than the atomic radius correspond to small potential energies.

B. Universal fit

The universal "KNGS" potential for antiproton atom interactions is given by

$$V_{\text{KNGS}}(r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r} \phi_{\text{KNGS}}(r/a_u), \quad (11)$$

where a_u is the screening length and

$$\phi_{\text{KNGS}}(x) = b_1 e^{a_1 x} + b_2 e^{a_2 x} + b_3 e^{a_3 x} + b_4 e^{a_4 x}. \quad (12)$$

From the fitting we found that the screening length resulting in the tightest grouping of the screening functions was

$$a_{u,\text{KNGS}} = \frac{2.80838}{Z^{0.373366} - 0.0112278}. \quad (13)$$

The parameters for the universal potential in eq. 2 are reported in table II. The a_i values are given in units of $1/\text{\AA}$ and the other fitted constants are unitless.

Fig. 3 shows that the change of the variable does not perfectly group the data, not even for the high-energy

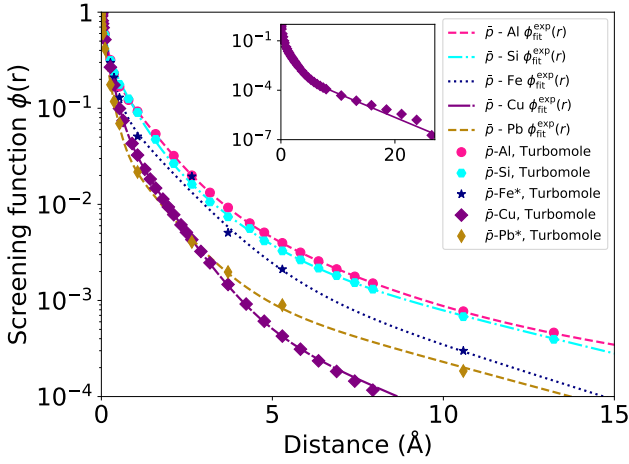


FIG. 2. The new screening functions with exponential fit and modified pair-specific screening functions with exponential fit. The asterisk (*) denotes data calculated at the relativistic level of theory. The graph is cropped at $\phi(r) = 10^{-4}$, since smaller values of the screening functions correspond to a potential energy approaching chemical energies. The insert shows the calculated data points and the exponential fit for Cu, where small values of the screening function are also shown.

TABLE II. The fitted parameters of the universal potential. The last linear coefficient is $b_4 = 1 - b_1 - b_2 - b_3$ to ensure that we obtain the physically correct limit. Headings X_n refer to the n -th term in the screening function. The errors were estimated using Jackknife estimate of standard error given by eq. 9.

	X_1	X_2	X_3	X_4
a	-24.8725	-1.30493	-0.286527	-4.53551
±	3.155	0.2267	0.04925	0.7006
b	0.14589	0.167284	0.00622113	$1 - b_1 - b_2 - b_3$
±	0.006426	0.01301	0.00150	
u	2.80838	0.373366	-0.0112278	
±	0.1031	0.01935	0.07507	

part of the potentials. The grouping seems to be less tight than for real-matter potentials [4].

The quantum chemical calculations for He, Li and W reported in Fig. 4(a) were performed after the universal potential was constructed, so they serve as a true test of the quality of the universal model. The tests of the universal potential for these calculated pair-specific values show that the obtained errors are of the same size as for the pair-specific potentials that were included in the fit, *cf.*, table I. For W the average error Δ_{univ} is ~ -6.9 , which is smaller than the error for Ne (~ 9.9) and of the same size as the error for Ti (~ -7.6). The root-mean-square error $E_{\text{rms,univ}}$ for W (~ 0.47) is actually smaller than the error for most of the elements that were considered in the fit. The errors for He and Li are of the same

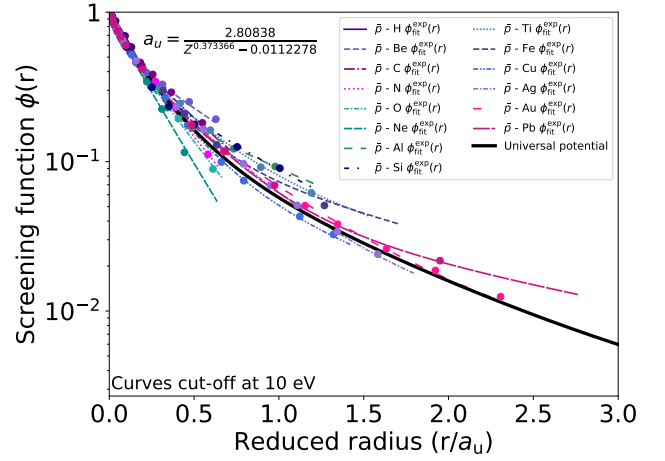


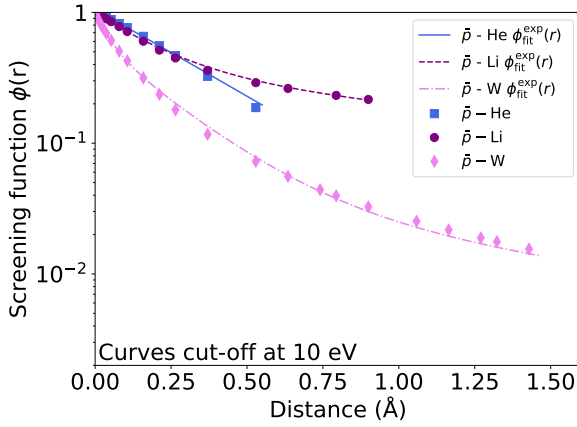
FIG. 3. The pair-specific screening functions plotted as a function of the reduced radius with the screening length given by eq. 13. The solid line is the universal potential. The quantum chemically calculated data for the pair-specific screening functions are shown with dots. For the pair-specific screening function and calculated data, only screening functions corresponding to a potential energy above 10 eV are included in the figure, since the universal potential could not reproduce well the interactions at lower energies.

size or smaller than the error for many of the elements included in the fit, which indicates that the universal potential can be considered to be a reasonable "average" potential for antiproton interactions with the nuclei of all elements. Fig. 4(b) shows the screening function for He, Li and W and the universal potential plotted as a function of the reduced radius.

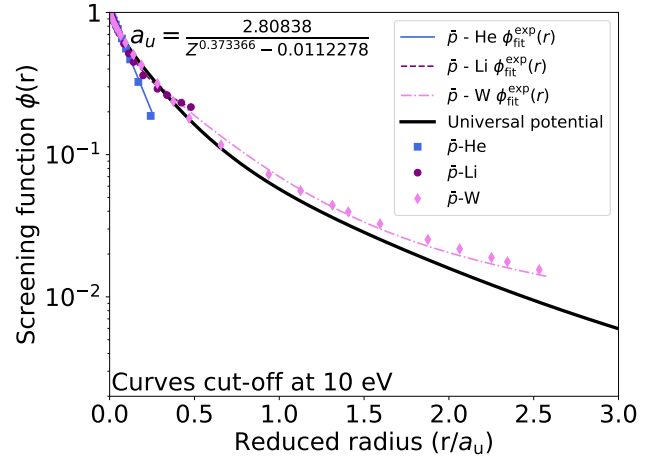
Our results show that a good fit with a single functional form depending on Z_2 can be achieved, with no obvious systematic deviations. This indicates that the screening of the antiproton charge depends mainly on the total electron density and its distance from the atom core. This is in spite of the outermost electron density of free atoms certainly having complex dependencies on the atomic number; however, as the screening depends on all the electrons, the wave functions of the outermost electrons do not lead to significant systematic deviations in the total screening.

IV. COMPARISON OF SCATTERING BEHAVIOR

To understand how significant the differences between the universal and pair-specific potential are in practical simulations, we first modeled the case of antiprotons scattering from a single free atom, which corresponds to an experimental situation of antiprotons scattering in a dilute gas of neutral atoms. The calculations were performed using molecular dynamics (MD) simulations as this enables the treatment of complex trajectories



(a) Pair-specific screening functions for He, Li and W.



(b) Screening functions for He, Li, W and the universal potential, as a function of the reduced radius.

FIG. 4. The screening functions for He, Li, W and the universal potential shown as a function of (a) the interatomic distance r , (b) the reduced radius r/a_u . The dots denote values obtained in the new quantum chemical calculations. The coefficients of the lines of the exponential fit are listed in table I. These data were not used when fitting the universal potential. Only screening functions corresponding to a potential energy above 10 eV are included in the figure. We use this cut-off to make the figure comparable to the other figures and since the universal potential in general does not reproduce well the interactions at lower energies.

[29, 30]. Electronic stopping was not included in these simulations as the scattering was treated in the elastic regime. In this case, the trajectories of the antiprotons around the nucleus are due to the purely attractive spherical potential. The scattering simulations were performed with the MDRANGE code [7, 31]. In the simulations, we used the KNGS screened Coulomb potential, eqs: 11, 12 and 13. The scattering was described classically, as quantum scattering effects become significant typically at MeV and higher energies [32].

Results for the Si- $\bar{p}$ scattering simulations at 1 keV are shown in Fig. 5. For understanding of how significant it is to use a specific antiproton potential, the figure shows (as in our earlier work [7]) comparisons with scattering simulated for a proton (p^*) and a hypothetical negative proton ($-p^*$) and interaction between an antiproton and an unscreened Si nucleus (denoted Coulomb*). The "negative proton" (i.e. the hypothetical case of a particle with the screening function of the proton but with negative charge) was included to show how strongly the difference in antiproton and proton screening is reflected in the experimentally significant scattering. The data shows that the scattering from Si for the true antiproton potentials is very different from that of a proton or a pure Coulomb potential, emphasizing the need to use actual antiproton potentials.

The figure also shows a comparison of scattering calculated for an implementation of the antiproton potential with numerical interpolation of the screening function ($\bar{p}^*$) and one directly calculated with the pair-specific analytical form ($\bar{p}$) given in eq. 2. There is a small dif-

ference between the numerical and analytical implementation results. This indicates that the scattering calculations may be sensitive to interpolations if implemented from a data point sets, and that whenever possible it is better to use an analytical implementation.

MDRANGE was also used to simulate elastic antiproton-atom collisions of various energies with an impact parameter b of 0.01 Å and 0.1 Å for different antiproton-atom pairs. The results of these simulations are shown in Fig. 6. The simulations were performed for antiproton-atom collisions with an initial kinetic energy of the antiproton in the range of 1 eV - 0.6 MeV. We repeated the simulations for all energies and impact parameters using the pair-specific potentials and the universal potentials.

As shown in Fig. 6, the differences in transmitted energy that were obtained in the simulations using the pair-specific potential and in the simulations using the universal potential are small. They are < 3 eV for all antiproton-atom collisions except for the antiproton collisions with H. For collisions with energies above 10 keV, the difference in transmitted energy is about ± 1 eV, which is completely negligible compared to the initial energy. The larger difference for H was expected because the universal screening function appears to be less accurate for H at longer internuclear distances, as shown in Fig. 3. The scattering results show that the universal potential describes the energy loss in binary collisions very accurately when compared to the pair-specific potentials, except possibly for the scattering from H at low energies.

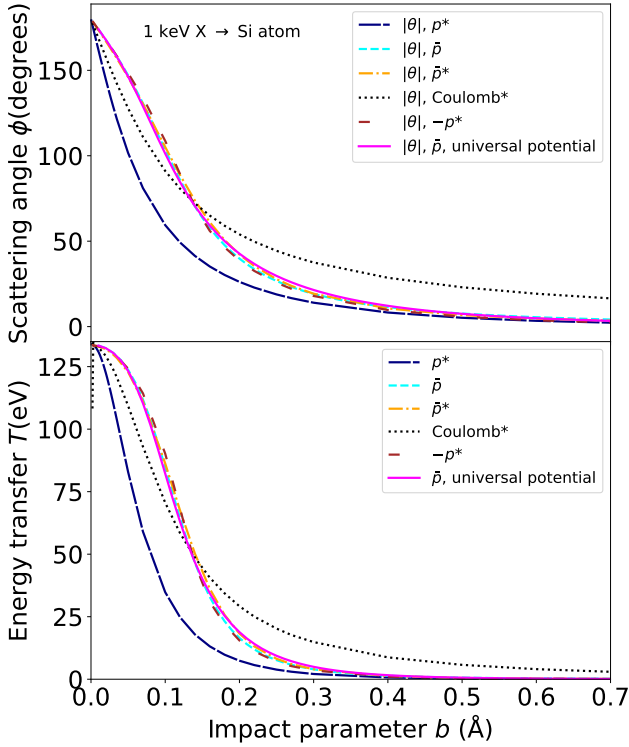


FIG. 5. The scattering angle and the energy loss of 1 keV antiproton $\bar{p}$ and proton p colliding with a single Si atom. For comparison, the scattering by a hypothetical negative proton ($-p^*$) and a pure Coulomb scattering (no screening function) is also shown. Data marked with an asterisk (*) denotes the same data as in Ref. [7]. The $\bar{p}^*$ data was calculated with a numerical cubic spline implementation of the potential and its derivative, whereas the $\bar{p}$ data uses an analytically calculated potential and derivative. The scattering angle θ has opposite sign for attractive and repulsive potentials. Here we have plotted the absolute value of the angle for easier comparison.

V. COMPARISON WITH EXPERIMENTS

To allow direct comparisons with experiments, we repeated previous MD recoil interaction approximation (MD-RIA) simulations [8] using the implemented analytical pair-specific and universal potentials. In the RIA approach, the passage of an ion (in this case the antiproton ion) in a material is modeled by describing all the interactions of the ion with nearby atoms of the sample using the molecular dynamics approach without calculating the interactions of sample atoms with the other sample atoms. Thus, only the ion-recoil interactions are included in the modeling. This approach has been shown to enable efficient description of the energy loss and movement path of ions in materials, while still not limiting the interaction to only the strongest atom collisions as in binary collision modeling [6, 33–35]. Moreover, it also has an advantage compared to the binary collision approximation [36] that the interatomic potential can also have an attractive part without introducing any ambiguities [37], which is crucial

in molecular dynamics simulations of antiprotons.

The simulations were carried out for (i) homogeneous polyethylene naphthalate (PEN, $C_{14}H_{10}O_4$), and (ii) a layered foil structure of Ag, biaxially-oriented polyethylene terephthalate BoPET ($C_{10}H_8O_4$), and Ag as in Ref. [8]. For all simulations using these foils, we simulated the antiproton beam by investigating one antiproton in the foil at a time, and repeating the simulation such that the energy spread of initial kinetic energy of the antiprotons was 5 keV. The simulations were repeated 10 000 times for all energies investigated. The electronic stopping was included in these simulations as a frictional force slowing down the antiproton in the direction opposite to its movement direction as in Ref. [8].

Fig. 7 shows the measured and simulated energy distribution of antiprotons transmitted through a 1800 nm thick BoPET foil with a 25 nm thick Ag coating on both sides. The average antiproton beam energy is 111.5 keV with an energy spread of 5 keV. The results of the simulations are compared to those obtained in a Penning trap experiment with the same setup [38]. The results of the simulations are normalized to the total number of incident antiprotons. The results obtained in the simulations with the universal potential barely differ from the ones obtained in the simulations using the pair-specific potential. Near the maximum transmission probability, the results obtained in the pair-specific potential simulations agree slightly better with experiment than with the results obtained with the universal potential.

Fig. 8 shows the relative intensity of the antiproton beam transmitted through a 1300 nm thick PEN foil as a function of the energy of the incident beam. The results of the simulations are compared to laser-spectroscopy measurements of $\bar{p}^4\text{He}^+$ [11]. The results of the simulations obtained using universal potential barely differs from the previously published results obtained in simulations using the pair-specific potential. To consider the possibility that antiprotons with a large off-normal exit angle are not detected in the experiment [8], we also report results for simulations in which antiprotons with an exit angle $\theta_{\text{exit}} > 50^\circ$ are not counted in the transmission yield.

Fig. 9 shows the results obtained in a Penning trap experiment, where the antiprotons are annihilated in a foil consisting of a 1800 nm thick BoPET layer with a 25 nm thick Ag coating on both sides. The total number of transmitted antiprotons is normalized to one. A uniform magnetic field of $B = 2.5$ T was applied perpendicularly to the surface of the foil [?]. We assume that antiprotons emerging from the foil with a lateral velocity component $v_\perp$ undergo a cyclotron motion with the Larmor radius given by

$$r_{\text{larmor}} = \frac{m_{\bar{p}} v_\perp}{eB}. \quad (14)$$

Following Ref. 8, we did not explicitly account for the effects of the magnetic field in the simulations. Instead, we assumed that the antiprotons with $r_{\text{larmor}} > 5$ mm

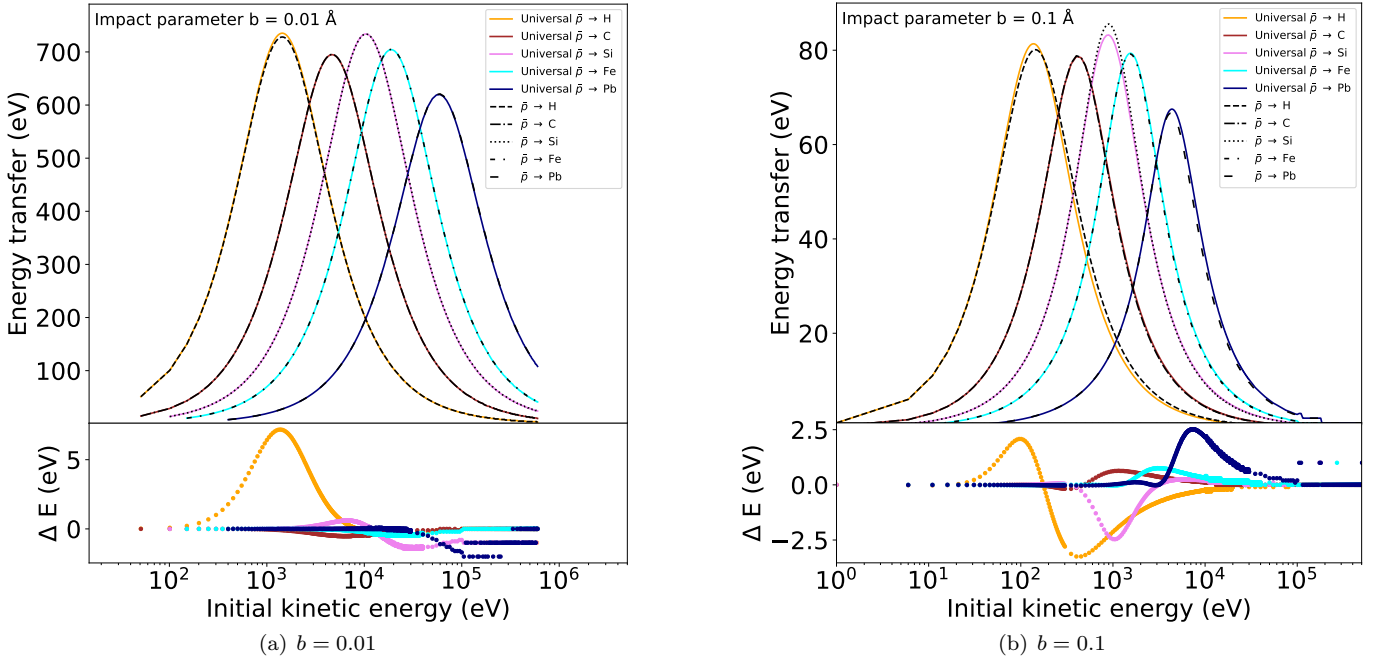


FIG. 6. The energy loss for an antiproton in elastic collision with an initially stationary H, C, Si, Fe or Pb atom as a function of the initial kinetic energy of the antiproton. The simulations are done with (a) impact parameter $b = 0.01$ and (b) impact parameter $b = 0.1$. The lower plot shows the difference in energy transmitted for simulations performed with the universal potential and with the pair-specific potential.

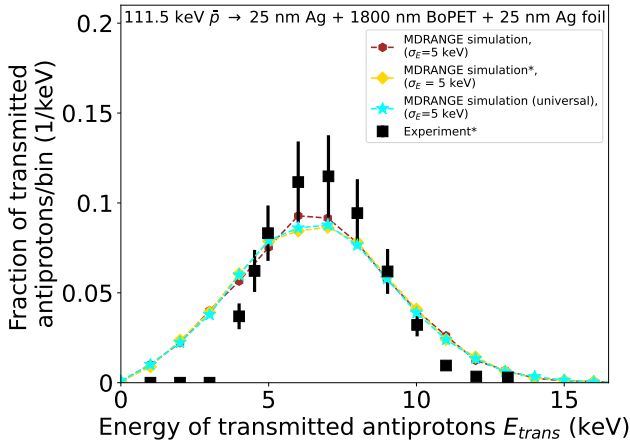


FIG. 7. The distribution of antiprotons with an incident energy of 111.5 keV emerging from a 1800 nm-thick BoPET foil with a 25 nm thick Ag coating on both sides. We repeated the simulations for 10 000 antiprotons with an energy spread of 5 keV using both the pair-specific and the universal potential. The experimental data (filled squares) are from Ref. 11. Data from Ref. [8] are denoted with *.

rapidly annihilate in the vicinity of the foil. The results obtained in the simulations with the universal potential barely differ from the ones obtained using the pair-specific potential.

The comparisons with experiments show that the results obtained with the simulations using the universal potential are almost identical to the results of the simulations performed with the pair-specific potential. They are also in good agreement with experimental data.

VI. CONCLUSIONS

We report quantum chemical pair-specific data for antiproton interactions with He, Li, Fe, W, and Pb and analytical potentials fitted to these data. We also develop a universal antiproton-atom potential which can describe the interaction between antiprotons and atoms of atomic number Z_2 . This universal “KNGS” potential describes the interactions with a single set of parameters as a function of the interparticle separation r and Z_2 . Comparisons to binary collision scattering simulations using these potentials to experimental data showed that the differences between the pair-specific and universal potentials are very small. Both potentials showed good agreement with the available experimental data. Since the universal potential is effectively an average, losing some of the fidelity of the pair-specific one, we recommend the use of the pair-specific simulations whenever they are available.

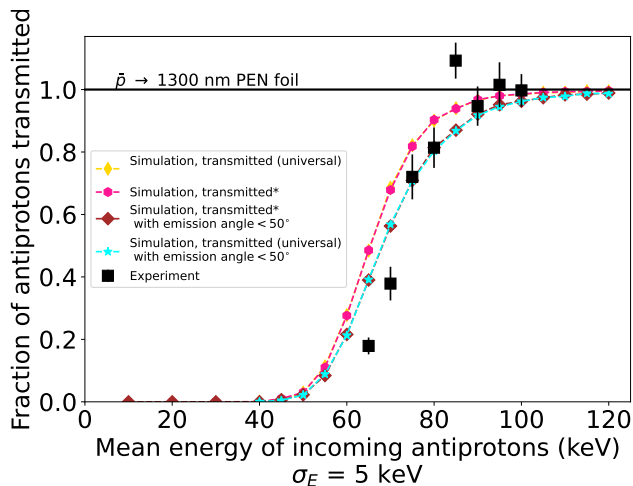


FIG. 8. The fraction of antiprotons transmitted through a 1300 nm thick PEN foil as a function of the energy of the incident beam. Results obtained in MD-RIA simulations that are performed using the universal interatomic potential and with the pair-specific interatomic potential are shown. The simulations were repeated 10 000 times with an energy spread of 5 keV for all simulated incident beam energies. Data from Ref. [8] are denoted with *.

DATA AVAILABILITY

Data sets, all final data used for the graphs and the software and script source codes are available at <https://doi.org/10.5281/zenodo.17953259> [39].

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Appendix A: Antiproton-atom interaction energies

The original quantum chemical data for He, Li, Fe, W and Pb are provided in tables III and IV. Data for the antiproton interaction with the positive Li^{1+} ion are also reported, which can be useful to estimate the effect of a charge state on the interaction.

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TABLE III. The interaction energy between an antiproton and He, Li, W atoms and positively ionized Li, calculated at the Hartree-Fock (He,Li,Li⁺) and scalar-relativistic Dirac-Fock (W) levels of theory.

Distance r (bohr)	Interaction energy			
	He (hartree)	Li (hartree)	Li ⁺ (hartree)	W (hartree)
10000000000.0	-2.859895425629	-7.432693104073	-7.236372525647	-16138.40318675
1000000.0				-16138.40318668
1000.0	-2.859895425628	-7.432693112990	-7.237372525599	-16138.40318668
100.0	-2.859895427877	-7.432693789589	-7.246372526461	-16138.40318648
50.0	-2.859895460825	-7.432704103485	-7.256372539344	-16138.40319861
45.0	-2.859895479785	-7.432709850619	-7.258594768905	-16138.40320451
40.0	-2.859895511968	-7.432719918542	-7.261372559486	-16138.40321567
35.0	-2.859895572787	-7.432738792970	-7.264944011361	-16138.40323645
30.0	-2.859895698240	-7.432777578369	-7.269705965324	-16138.40327942
25.0	-2.859895991163	-7.432867583357	-7.276372746549	-16138.40337856
20.0	-2.859896806546	-7.433115145366	-7.286373064862	-16138.40365016
19.0				-16138.40375312
18.0				-16138.40388625
17.0	-2.859898071899	-7.433491598057	-7.295197087991	-16138.40405932
16.0	-2.859898799424	-7.433704106590	-7.298873843244	-16138.40428903
15.0	-2.859899793142	-7.433991076235	-7.303040898924	-16138.40459804
14.0	-2.859901180993	-7.434385955314	-7.307803348274	-16138.40502179
13.0	-2.859903166897	-7.434941674585	-7.313298636131	-16138.40561501
12.0	-2.859906087949	-7.435744202974	-7.319710048692	-16138.40646524
11.0	-2.859910528955	-7.436933083681	-7.327287566120	-16138.40771823
10.0	-2.859917570609	-7.438728227269	-7.336381241169	-16138.40961999
9.0	-2.859929390414	-7.441466456163	-7.347496887329	-16138.41261381
8.0	-2.859950398132	-7.445675260332	-7.361393673916	-16138.41753697
7.0	-2.859988862154	-7.452255421354	-7.379265649282	-16138.42607703
6.0	-2.860066808940	-7.462887252224	-7.403105918758	-16138.44186465
5.5				-16138.45477820
5.0	-2.860260538293	-7.480852757005	-7.436511120562	-16138.47339777
4.7				-16138.48857299
4.4				-16138.50797217
4.2				-16138.52395870
4.0	-2.861022066702	-7.513101257030	-7.486709951549	-16138.54305985
3.7	-2.861692179107	-7.527607646320	-7.507103036516	-16138.57928282
3.5	-2.862404981405	-7.539117106676	-7.522660824417	-16138.61005064
3.4				-16138.62795511
3.2	-2.864120049596	-7.559901625345	-7.549691758379	-16138.67000335
3.0	-2.865914011203	-7.576706000496	-7.570764404846	-16138.72249077
2.7	-2.870172832030	-7.607770744377	-7.608355390215	-16138.82872478
2.5	-2.874623117372	-7.633584762151	-7.638575772392	-16138.92592689
2.4				-16138.98550535
2.2	-2.885457965917	-7.683056995449	-7.694677938243	-16139.13446280
2.0	-2.897365806208	-7.726049753470	-7.742056068317	-16139.33910935
1.7	-2.928836912709	-7.813825688250	-7.836244349573	-16139.82324287
1.5	-2.966782251512	-7.896578941589	-7.923065255329	-16140.35792369
1.4				-16140.73305990
1.2	-3.079565177072	-8.088174652654	-8.120220076295	-16141.83995179
1.0	-3.234315727231	-8.303786130794	-8.338995122680	-16143.78102229
0.7	-3.787099912745	-8.978554503791	-9.017318096826	-16150.75363157
0.5	-4.729189680773	-10.12312695841	-10.16330783947	-16165.02496973
0.4	-5.640831138227	-11.29406518757	-11.33470260726	-16182.11821473
0.3	-7.233490434311	-13.45735002180	-13.49835009788	-16216.36169620
0.2	-10.51167834365	-18.14778816664	-18.18912449760	-16296.18152121
0.15	-13.82604265973	-23.01784733745	-23.05934400313	-16387.61159105
0.1	-20.48045092110	-32.91396554382	-32.95558933727	-16590.43292801
0.07	-29.04776956470	-45.72481596462	-45.76647811364	-16868.93732830
0.05	-40.47477539548	-62.84481744981	-62.88647991149	-17257.54919506
0.04	-50.47430573835	-77.83602201775	-77.87767488610	-17606.94925060
0.03	-67.14070602767	-102.8290836687	-102.8707174741	-18198.91050991
0.02	-100.4739761062	-152.8240851244	-152.8656817038	-19399.22036916
0.015	-133.8073453559	-202.8223420285	-202.8639063414	-20610.62756785
0.01	-200.4740740476	-302.8211237161	-302.8626411987	-23050.69468088
0.007	-286.1883979059	-431.3920781823	-431.4335612814	-26204.34922398
0.005	-400.4741334463	-602.8204383476	-602.8618985869	-30421.01088965
0.004	-500.4741420279	-752.8203624954	-752.8618124258	-34115.32725274
0.003	-667.1408156135	-1002.820305254	-1002.861746312	-40276.71123738
0.002	-1000.474154024	-1502.820265511	-1502.861699693	-52605.41723279
0.0015	-1333.807489162	-2002.820251859	-2002.861683516	-64936.79668113
0.001	-2000.474157126	-3002.820242196	-3002.861672009	-89601.83883210
0.0007	-2857.617014796	-4288.534523991	-4288.575953036	-121315.3495177
0.0005	-4000.474157906	-6002.820236437	-6002.861665123	-163600.6499255
0.0004	-5000.474158001	-7502.820235746	-7502.861664300	-200600.4791130
0.0003	-6667.140824741	-10002.82023521	-10002.86166366	-262267.0026621
0.0002	-10000.47415813	-15002.82023483	-15002.86166320	-385600.2241662
0.00015	-13333.80749148	-20002.82023470	-20002.86166304	-508933.5149714
0.0001	-20000.47415816	-30002.82023460	-30002.86166293	-755600.1496023

TABLE IV. The interaction energy between an antiproton and Fe, Pb atoms calculated at the scalar-relativistic Dirac-Fock level of theory.

Distance r (bohr)	Interaction energy	
	Fe (hartree)	Pb (hartree)
0.0	-1157.27075294294	-20243.78434985441
0.0001	-261157.27097314436	-840243.7485763967
0.0002	-131157.27178346418	-430243.87913389126
0.0005	-53157.27949521972	-184244.6546377461
0.0007	-38300.1395088604	-137388.22210956196
0.001	-27157.29889152299	-102246.68591146404
0.002	-14157.37269880475	-61252.44550771211
0.005	-6357.83796204596	-36675.54356842563
0.007	-4872.60360421745	-32006.34731593262
0.01	-3759.23729706619	-28515.53103408991
0.02	-2463.28129792932	-24474.92973778712
0.03	-2034.86803146506	-23146.96690299799
0.05	-1697.45603511142	-22107.82658125929
0.07	-1556.41962647791	-21679.90255364297
0.1	-1453.31729937645	-21372.82326640215
0.2	-1340.41797727459	-21050.8004339609
0.5	-1286.70015689397	-20908.99117056067
0.7	-1278.99680628618	-20893.94052512832
1.0	-1274.59837688238	-20885.84553347554
2.0	-1271.89875739493	-20881.0491374538
5.0	-1271.33871589612	-20880.22494691328
7.0	-1271.25600169379	-20880.18146381307
10.0	-1271.24266983737	-20880.16565615267
20.0	-1271.23756653063	-20880.15907568554
30.0	-1271.23724098249	-20880.15849748677
50.0	-1271.23717765398	-20880.15831915951
1000000.0	-1271.23716110855	-20880.15827345484

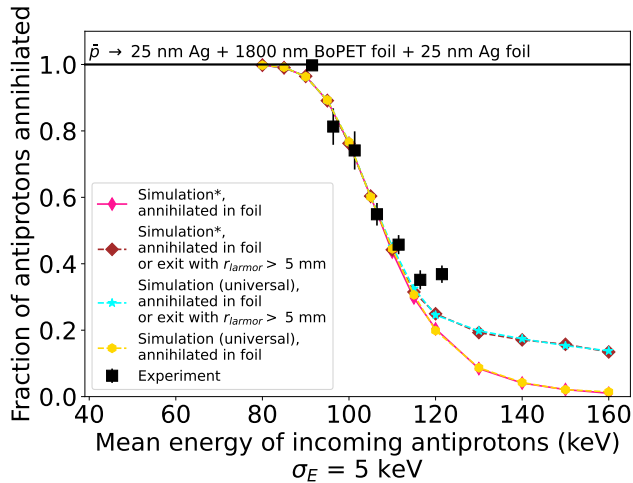


FIG. 9. The fraction of antiprotons annihilated in a 1800 nm thick BoPET foil with a 25 nm thick Ag coating on both sides as a function of incident beam energy. The MD-RIA simulations are performed with the universal interatomic potential and with the pair-specific interatomic potentials. For all incident beam energies we simulated, the simulations were repeated 10 000 times with an energy spread of 5 keV. The asterisk (*) denotes simulations that were performed using pair-specific potentials.

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